Computers and Fluids 000 (2018) 1–21

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Investigation of adaptive design variables bounds in dimensionality reduction for aerodynamic shape optimization

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ARTICLE INFO

Article history:
Received 20 December 2017
Revised 11 July 2018
Accepted 16 July 2018
Available online xxx

MSC:
00-01
99-00

Keywords:
Design space reduction
Aero shape optimization
Proper orthogonal decomposition
Curse of dimensionality
Geometric filtration

ABSTRACT

Geometric filtration with Proper Orthogonal Decomposition has been demonstrated in the last decade, promising effective in reducing the design space dimensionality for several industrial shape optimization problems. Thanks to the capability of re-ordering the data according to decreasing variance, the Proper Orthogonal Decomposition (POD) extracts and filters the basic features of the dataset so as to formulate the optimization problem into a new, shrunk design space. The paper proposes and investigates the reduction of the search hyperspace volume thanks to the application of POD to a set of design solutions in on-line optimization: in particular, the combination of a selection algorithm and the re-computation of the POD modes while the optimization is progressing is studied. A series of optimization results are shown for a two–dimensional test case by using a genetic algorithm. Both native geometry parameterization and the filtered one are used to highlight benefits and drawbacks of the proposed approach. Results show that, by employing the filtered parameterization and by properly/adaptively adjusting the bounds of the reduced design space, it is possible to achieve and even enhance the design performance attained with the native parameterization.

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1. Introduction

In the framework of global optimization approaches for aerodynamic design, a shape is usually parameterized by acting on the design variables (DV) whose number and bounds generate the design space. However, when increasing the geometry complexity of the problem at hand, the number of design variables may grow up significantly, giving rise to the well-known 'curse of dimensionality' [1].

This may hamper the success of the optimization process, as large design spaces may lead to multi-modal and noisy landscapes. As a consequence, the problem of searching for a global solution may result hard or even intractable, independently of the search method, i.e. deterministic or stochastic or meta–heuristic.

In surrogate-based optimization (SBO), the meta–model that mimics the behavior of the objective function is made explicitly dependent on the design variables. From literature, it is known that, whatever the meta–model, a loss in prediction quality is associated to an increase of dimensionality [2]. On the other hand, sensitivity analysis often shows that not all the design variables have the same influence on the objective function behavior. As a matter of fact, a reduction of the design space is envisaged to preserve the main features of the target function landscape while avoiding the high–dimensional noise.

Another issue is related to the huge amount of CPU required to face with an industrial aerodynamic design. Indeed, geometric complexities and non-linear flow features (e.g., flow separation, shock waves, shock–boundary layer interaction) still require to use fine mesh size and large number of CFD iterations to be correctly solved. An even more crucial bottleneck is represented by the search of a solution with a global algorithm, which may require a large number of CFD evaluations. Therefore, it is mandatory to reduce the problem complexity at each level of the design chain by means of the parallelization of the CFD solver, the usage of surrogate or reduced order models to evaluate the objective function and the reduction of the design space.

In literature, design space reduction (DSR) is treated with different strategies to shrink the bounds of the search volume like trust region approaches [3], heuristic, move limits [4], Variable-Complexity Response Surface Modeling Method (VCRSM), and Concurrent Sub Space Optimization (CSSO) [5]. For example, VCRSM as proposed by Zahir [6] suggests a preliminary exploration of the design space with a low fidelity model, then selects the new reduced

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https://doi.org/10.1016/j.compfluid.2018.07.012
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bounds with a pattern search coupled with high fidelity simulation and integration of data. CSSO is a subspace coordination procedure: here the data generated by the subspace optimizers is not uniformly centered about the current design, but instead follows the descent path of the subspace optimizers [5,7]. The common feature of these techniques is the reduction of the search volume and the associated relieving effect, mostly if the optimization is driven by surrogate models.

In another perspective, DSR can be viewed also as a reduction of the inherent dimensionality of the problem, i.e. a technique to identify a lower dimension that effectively and efficiently drives the problem at hand. The aim is to learn from a given sampling set of the original design space and to map it to a lower dimensional space while keeping the most important features of the original design problem. Various strategies have been proposed in literature to seek an equivalent lower dimensional representation, even if some losses are introduced. Proper orthogonal decomposition (POD), kernel POD, locally linear embedding, Laplacian eigenmaps, isomap and semidefinite embedding are just some examples [8–10].

In aerodynamics, Robinson and Kean [11] used Gram-Schmidt orthogonalization to define an airfoil parameterization with orthonormal basis functions derived from a small database of supercritical airfoils. Successively, Toal et al. [12] introduced the geometric filtration by means of POD in the context of aerodynamic shape optimization (ASO): the design variables set were filtered by performing a variance analysis based on Proper Orthogonal Decomposition. Exploiting the intrinsic properties of POD, the geometric data are re-arranged and ranked according to their relative importance, thus deriving a new parameterization in a transformed space. The beneficial aspect of this transformation is two–fold as it brings a quantitative and qualitative filtering at the same time: first, as a result of POD ranking and truncation, the new design space is shrunk and the effective size of the problem at hand is reduced (quantitative filtering); second, the new geometric modes are orthogonal and, hence, independent : this removes all possible spurious coupling between original design variables [12] (qualitative filtering). Poole [13,14] collects a database of airfoils and then filter them according to performance indexes and to the optimization problem. A geometric inverse problems was set to demonstrate the extent to which the reduced DVs are able to recover arbitrary airfoil shapes. In particular, he states that it is possible to represent a wide variety of airfoils geometries within a small tolerance also with eight reduced DV, furthermore he recommends that a wide range of airfoil shapes is essential to ensure an efficient coverage of the design space of a variety of sections. A major role is played by the sample density in that both minor surface and large topology changes can be captured effectively. Masters et al. [15] compare seven different airfoil parameterizations and state that SVD methods give better results in terms of efficient coverage of design space in the reconstruction of 2000 geometries belonging to a large database. POD (or PCA) was also used in active subspace method (ASM) [16] to discover and exploit low-dimensional and monotonic trends in the objective space as a function of the design variables. The method is based on the evaluation of the gradient. In the field of hydrodynamic optimization, Diez et al. [17,18] employed PCA to reduce the dimensionality of the problem, facing also with multiple design conditions. They add both physics–based lumped or distributed parameters in the design modification vectors. To obtain this parameter a preliminary low-fidelity analysis is performed. In a recent work [19], the authors compare linear PCA reduction technique, with non-linear technique like deep-autoencoder (DAE, a non-linear extension of PCA): here they showed the superior compression quality of DAE, with optimization results lightly better than PCA. Concerning the study of reduced variable bounds and how to set them, literature findings show that the upper and lower bounds of the new reduced variables are often chosen as the minimum and maximum values of the POD coefficient vectors [12,17]. Li et al. [20] introduce a different strategy, where the first two modes coefficients are taken with min/max criterion, while the others are smoothed and scaled with a percentage (10%) of their variance. They set up a surrogate-based optimization approach employing a database of 2000 airfoils, a gradient-enhanced Kriging model (GE-KPLS) as surrogate and a gradient-based approach (SNOPT) as optimizer. A reduced parameterization is introduced for mean line and camber distribution separately. Optimization results are relative to subsonic and transonic optimizations, comparing the outputs of SBO with ADflow, both in reduced Design Space. In this case a comparison with the native DS is not possible since they have deduced the reduced parameterization from an existing dataset of airfoil shapes.

The present authors already proposed the application of the DSR technique to two- and three-dimensional surrogate-based optimization: in particular, in the first investigation [21] the optimization of an airfoil in subsonic viscous flow was studied; in the second [22], the DSR was applied to an industrial case, i.e. a wing shape optimization in multi-point, transonic and viscous conditions. The last application represented quite a novelty with respect to recent papers [23–25]. In this perspective, the present paper represents a step inwards the full understanding of the potential and exploitation of the POD-based design space reduction method. Indeed, the paper deals with the study of the bounds of the reduced parameterization and, consequently, the effect of varying the design space volume within a shape optimization problem. A more pronounced emphasis is put on a twofold aspect: on one hand, the reduced design variables setting and adaptation during the optimization process, thus adjusting the reduced basis with the ongoing search results; on the other hand, addressing the low dimensional mapping in a more local sense, that is driving it to promising and narrow regions of the reduced design space. Both improvements are effective in confining the randomness and mitigating the dispersion of the initial geometry database, obtained through a pseudo–random Latin Hypercube Sampling. The paper is organized as follows: the next section will provide details about the DSR technique based on POD; afterwards, the optimization process and the POD basis updating strategy are presented; finally, a quite extensive section is devoted to the presentation of the results and to the critical discussion.

2. Geometric data reduction by POD

Proper Orthogonal Decomposition is a technique to compute a linear basis of vectors which is optimal in some sense. In other words, it provides the best representation of a given dataset in a different reference frame originated by the POD basis vectors. A detailed mathematical formulation for the derivation can be found in [26,27]. Here, the fundamental concepts and relations are recalled. The dataset is organized in a snapshot matrix $\mathbf{S} = \{S_1, S_2, \ldots, S_n\}$, which collects the available data in a column–wise manner, where n is the number of experiments or numerical simulations. Here, it is assumed that each snapshot element S_k is obtained by varying a set of parameters $\mathbf{w} = \{w_1, \ldots, w_m\}$ which, in the present case, represent the design variables of the optimization problem at hand. The combination of the sets $\{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_n\}$ and $\{S_1, S_2, \ldots, S_n\}$ represent the so-called training dataset of database.

Computing a POD basis consists in searching a set of orthonormal vectors $\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_n$ such that the following relation holds:

$$S_j = \bar{S} + \sum_{i=1}^{n} \alpha_i(\mathbf{w}_j)\phi_i = \bar{S} + \sum_{i=1}^{\hat{n}} \alpha_i(\mathbf{w}_j)\phi_i + \epsilon_{\hat{n}}^j = \bar{S} + \sum_{i=1}^{\hat{n}} (S_j, \phi_i)\phi_i + \epsilon_{\hat{n}}^j$$

where $\bar{S}$ is a base solution [27,28] (i.e. an average field), the scalars α_i are the unknown POD coefficients, $\hat{n} \le n$ and the error $\boldsymbol{\epsilon}$ is "optimal", i.e. the

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